Indian J. Phys. **68B** (5), 389 – 397 (1994)

I J P B
— an international journal

Elastic scattering of positron by alkali atom lithium

P K Verma
Department of Physics, L S College, Muzaffarpur-842 001, Bihar, India
and
D N Roy
Department of Physics, Patna University, Patna-800 005, Bihar, India

Received 10 June 1994, accepted 17 August 1994

Abstract : The modified form of Born approximation has been employed to calculate differential cross sections for elastic scattering of positrons by alkali atom lithium, in the energy range 100 eV–550 eV. Attempts have been made to extend and improve the Born approximation by taking into account the effect of nuclear interaction terms in the form of distorted wave (screened Coulomb waves). To study the impact of polarization effect, differential cross sections have been calculated with and without polarization potential The first Born approximation cross sections have been reported. The agreement between the present results and corresponding theoretical predictions in the literature are fair

Keywords : Elastic scattering of positron, differential cross section, distorted wave method, polarization potential

PACS Nos. : 34.40.+n, 34 80 Bm, 25 30 Hm

1. Introduction

At lower energies, there are some good variational methods to investigate positron-atom scattering, especially for hydrogen and helium. In the case of lithium, recently watts and Humberston [1] has investigated a low energy scattering using variational technique. However, in his calculation lithium has been considered as one-electron-target. At high energies, there are some good perturbative methods which predict reliable results. This is a challenge to theoretical physicists to find the suitable method to investigate this problem at medium energy. This is due to the fact that a large number of channels including continuum are open at intermediate energies. It is very difficult in practice, to include the effect of all channels including continuum in calculations. Literature reveals that some suitable distorted-

wave method is the bridge between low energy approximations and high energy approximations. There are different variants of distorted-wave methods that has been employed to investigate electron-atom and positron-atom scattering. All the dynamics of the system cannot be accommodated in a single distorted-wave method. Theoretical physicists have developed distorted-wave method according to the requirement of the problem. However, a suitable distorted-wave method that accounts for the effect of higher excited states and continuum is required to predict the observed cross sections.

It is wellknown that the effects of continuum are of key-importance in predicting the scattering parameters at low and medium energies. Keeping this in mind, we have used the distorted-wave method in which the effects of continuum are taken into account partially. In our distorted-wave model, we included a part of Coulomb potential in continuum wave function in the initial channel. The present method is the admixture of two methods, Coulomb-projected Born approximation and the method of Junker 1975 [2]. It is better than the Coulomb-projected Born-approximation in the sense that incoming positron does not see the bare nuclear charge. Instead, incoming positron will see an effective charge, screened due to the presence of target electrons. Therefore, the strong singularity that is present in Coulomb-projected Born-approximation is partially avoided. Lithium is the first member of alkali series, its valence electron is lossely bound. As a consequence, dipole polarizability of lithium is approximately 36.4 times more than that of hydrogen. Therefore, calculations carried out for positron-lithium atom scattering without explicit inclusion of dipole polarization is not worth-doing. We may further mention that 98% of polarizability of lithium atom comes from $2p$-state. By including the polarization potential in our calculation, we are including $L = 1$ excited state partially. Moreover, the effect of continuum in the present model is taken *via* distorted continuum wave function.

2. Theory

The Hamiltonian H for the positron-alkali atom can be expressed as

$$H = \left[-\left(\frac{1}{2}\right)\nabla^2_{r_1} - \left(\frac{1}{2}\right)\nabla^2_{r_2} - \frac{1}{r_1}\right] + \left[\frac{1}{r_2} - \frac{1}{r_{12}}\right]. \tag{1}$$

In the centre of mass reference frame $\bar{r}_1$ and $\bar{r}_2$ are the position vectors of the atomic electron and the incident positron with respect to the screened nucleus of target atom. $\nabla^2_{r_1}$ and $\nabla^2_{r_2}$ are the kinetic energy operators. Atomic units have been used throughout.

The Hamiltonian H is partitioned and expressed as

$$H = H_1 + W \tag{2}$$

with $$H_1 = H_0 + U, \tag{3}$$

where $$U = \delta / r_2, \tag{4}$$

$$W = (1 - \delta)/r_2 - \frac{1}{r_{12}}, \tag{5}$$

δ = Screening parameter,

and H_0 = Free Hamiltonian.

The functions ϕ_r, χ_r and ψ_r satisfy the following Schrödinger equations with Hamiltonian H_0, H_1 and H respectively.

$$\left.\begin{aligned} H_0\phi_r &= E_r\phi_r, \\ H_1\chi_r &= E_r\chi_r, \\ H\psi_r &= E_r\psi_r. \end{aligned}\right| \tag{6}$$

Let the system move from the initial bound state $|i\rangle$ with momentum $\bar{K}_i$ to the final state with momentum $\bar{K}_f$. Then the T-matrix elements can be expressed as

$$T_{i\to f} = \left\langle \phi_f \middle| V \middle| \psi_i^{(+)} \right\rangle, \tag{7}$$

where $$V = \frac{1}{r_2} - \frac{1}{r_{12}}. \tag{8}$$

Here, $\psi_i^{(+)}$ can be expanded with respect to H_1.

$$\psi_i^{(+)} = \sum_{n=0}^{\alpha} \left(G^{(+)}W\right)^n \chi_i^{(+)} \tag{9}$$

where $G^{(+)}$ is the Green function for H_1.

It would not be a crude approximation to retain only the first order term in the above expression, if we assume W to be a weak potential. Then the T-matrix element can be expressed as

$$T_{i\to f} = \left\langle \phi_f \, |V| \, \chi_i^{(+)} \right\rangle. \tag{10}$$

In atomic unit, differential cross section is

$$\frac{d\sigma}{d\Omega} = \frac{\mu^2}{4\pi^2} \frac{K_i}{K_f} |T|^2. \tag{11}$$

In present case, wave functions have been taken in the following forms

$$\phi_r = \exp(i\bar{K}\cdot\bar{r}_2)\,\phi_{nlm}(\bar{r}_1) \tag{12}$$

and $$\chi_i^{(+)} = \Gamma(1 + ia)\exp\left(i\bar{K}\cdot\bar{r} - \frac{\pi a}{2}\right)$$

$$\times {}_1F_1(-ia;1;iK_ir_2 - i\bar{K}_i\cdot\bar{r}_2)\phi_{nlm}(\bar{r}_1) \tag{13}$$

where $$a = \frac{\delta}{K}.$$

Here, $\bar{K}$ is the momentum for the direct channel, in which distortion is introduced. The screening parameter δ is evaluated following the method of Junker [2].

This method includes a part of Coulomb potential in incident continuum wave function. Physically, the effect of continuum is taken into account partially.

The radial part of atomic wave function for lithium is expressed as (Hartree-Fock wave function) follows :

$$\phi_{20}(r) = \sum_{i=1}^{2} a_i r \exp(-b_i r) + \sum_{i=3}^{6} a_i r^2 \exp(-b_i r). \tag{14}$$

(in ground state)

Now, T-matrix can be expressed in the form

$$T_{i\to f} = MF' \left[I_0 + \sum_{i=1}^{2} \sum_{j=1}^{2} N_{ij} \frac{\partial^2 I}{\partial \lambda_{ij}^2} + \sum_{i=1}^{2} \sum_{j=3}^{6} N_{ij} \frac{\partial^3 I}{\partial \lambda_{ij}^3} + \sum_{i=3}^{6} \sum_{j=3}^{6} N_{ij} \frac{\partial^4 I}{\partial \lambda_{ij}^4} \right] \tag{15}$$

In above expression

$$\bar{q} = \bar{K}_i - \bar{K}_f, \tag{16}$$

$$MF' = \Gamma(1 + ia) \exp\left(-\pi \frac{a}{2}\right),$$

$$\lambda_{ij} = (b_i + b_j),$$

$$N_{ij} = \left(-\frac{1}{4\pi}\right) a_i a_j, \tag{17}$$

$$I = \int\int \exp(i\bar{q}\cdot\bar{r}_2)\ {}_1F_1\left(-ia;1;iK_i r_2 - i\bar{K}_i\cdot\bar{r}_2\right) \exp\left[-(b_i + b_j)r_1\right] \left(\frac{1}{r_{12}}\right) d\bar{r}_1\, d\bar{r}_2, \tag{18}$$

and

$$I_0 = \int \exp(i\bar{q}\cdot\bar{r}_2)\ {}_1F_1\left(-ia;1;i K_i r_2 - i\bar{K}_i\cdot\bar{r}_2\right) \frac{1}{r_2} d\bar{r}_2. \tag{19}$$

Using Nordsieck-method [3], integrals involved in eq. (15) are evaluated and differential cross sections are calculated using eq. (11).

In present case, the asymptotic form of the polarization potential is $V_p = \left(-\frac{\alpha}{2r^4}\right)$ where α is the dipole polarizability.

The differential cross sections were calculated with polarization potential (DCSPP) and without polarization potential (DCSWP) so that effect of introducing polarization potential may be properly analysed.

3. Result and discussion

Distorted wave method has been designed to give results in intermediate energy range. In this energy range, infinite number of channels are open and effect of loss of inelastic flux is not negligible. It has been found in literature that positronium formation cross section for positron-alkali atom scattering is very high at low energy. With the increase of energy, capture cross section decreases very rapidly. As a result, the effect of capture channel on direct channel is not expected to be appreciable. The valence electron of alkali atom is loosely bound, so the effect of polarization is very significant. Considering this fact, we have performed the distorted wave calculation that takes account of polarization.

In Figures (1–6), the curve A represents values of the differential cross sections calculated by employing the distorted wave method without polarization (DCSWP). The curves B and C represent values of differential cross sections calculated by employing the first Born approximation (DCSB) and the distorted wave method with polarization (DCSPP) respectively. To ascertain the lowest energy at which the present distorted wave approach is expected to be valid, we present the results at energies from 100 eV to 550 eV.

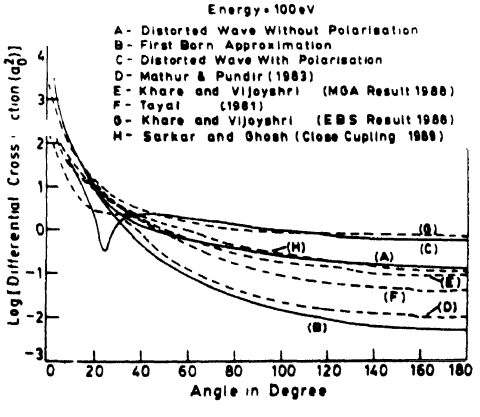

Figure 1. Differential cross sections for e^+–Li elastic scattering at 100 eV

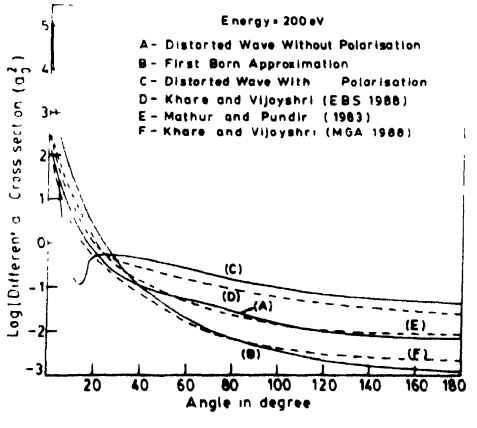

Figure 2. Differential cross sections for e^+–Li elastic scattering.

Present differential cross section with polarization (DCSPP) at all energies have provided a structure. The position of minimum shifts with change in energy. At 100 eV, it is around the scattering angle 21° (Figure 1), whereas at 550 eV the corresponding position of

minimum is around the scattering angle 10° (Figure 6). Thus we see that with enhancement of energy, the position of minimum is shifted towards forward angles.

The probable reason for structure in differential cross sections is the cancellation between the polarization potential and static potential.

At 100 eV, our present results with polarization are close to the EBS-results of Khare and Vijayshri [4] at large angles, whereas their MGA-results lie below our present set of results. Khare and Vijayshri have employed eikonal-Born series and modified Glauber approximation. In both methods, they have however, calculated second Born term in very simplified way. It amounts to include partial polarization.

Though Tayal *et al* [5] have carried out calculations in corrected static approximation and in an approximation, which is a combination of non-static part of higher order ($n \geq 3$) terms in Glauber amplitude with corrected static approximation but their results lie below our present set of results and those of Sarkar and Ghosh [6] Present results without polarization are close to those of Sarkar and Ghosh. They have applied five-state close-coupling approximation. Figure 1 displays these features.

At 200 eV energy of incident positron, two sets of results (MGA- and EBS-results) presented by Khare and Vijayshri [4] include the effect of polarization partially (Figure 2). As a consequence both results near forward direction are less than the first Born predictions. The effect of polarization in the present case, reduces the cross section near the forward direction. At larger angles of scattering, EBS-results favour the present results with polarization, while MGA-results are close to those of the first Born approximation. The result of Mathur and Pundir [7] are close to the present distorted wave without polarization-results.

Moreover, all curves have common tendency of merging together at the scattering-angle closer to zero. It is to be quoted that below 30° angle of scattering, the nature of variation is almost the same and they get closer and closer as one moves from 30° to 0°. It is a clear evidence that present results are justified and present approach is a suitable one.

As the energy of incident positron increases the differences between DCSPP and DCSWP and the same between DCSPP and DCSB decreases. Near forward direction DCSPP decreases exponentially but at large angles of scattering the slope of DCSPP is very small.

From 300 eV and above (Figures 3 and 4), at larger scattering-angle, difference between DCSB and DCSWP decreases. However, our polarization-results DCSPP at all energies are always higher than other two sets of results at larger angles of scattering. On the other hand at small scattering angle, the present results with polarization DCSPP are less than those without polarization DCSWP and the first Born results. This is due to cancellation between polarization potential and static potential. Our results with polarization always predict a minimum, whose position is shifted slightly towards forward angle with increase in energy

of incident positron. This structure in curve has been noticed by Ward *et al* [8] and Sarkar and Ghosh [6] also.

The present results with polarization predict higher values of DCSPP than DCSWP and DCSB. Sarkar and Ghosh [6] using five-state close coupling approximation predicted higher values at larger scattering angles.

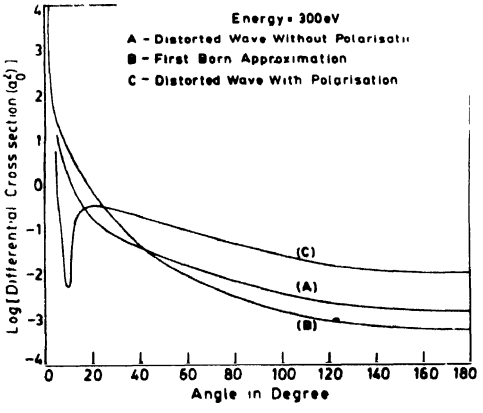

Figure 3. Differential cross sections for e^+–Li elastic scattering at 300 eV.

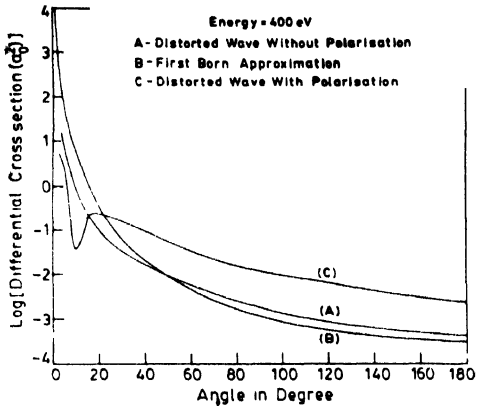

Figure 4. Differential cross sections for e^+–Li elastic scattering at 400 eV

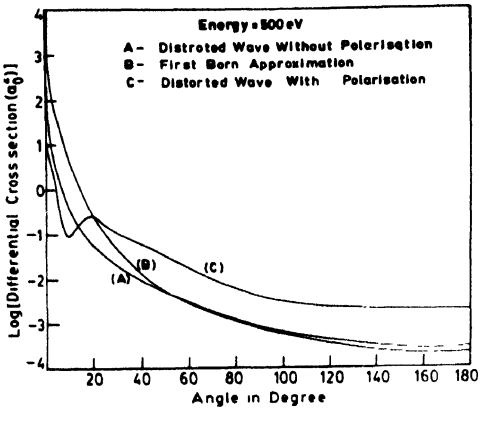

Figure 5. Differential cross sections for e^+–Li elastic scattering at 500 eV.

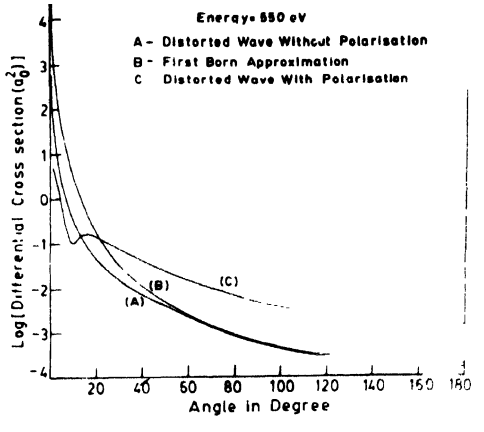

Figure 6. Differential cross sections for e^+–Li elastic scattering at 550 eV

Considering all the observations, the present values of differential cross sections at all scattering angles are expected to be reliable.

Figures 5 and 6 show curves at 500 eV and 550 eV respectively. One feature is visible at 500 eV, that is, the curves B and A are closer at all scattering angles. This

shows agreement between the distorted wave without polarization-results and the first Born-results.

At 550 eV the closeness between B and A curves has further improved. This confirms above agreement between DCSWP and DCSB, which was expected in the results of present approach.

At both energies DCSPP and DCSWP have separation in their corresponding values at larger scattering angles. The larger values of DCSPP at larger angle of scattering are due to the effect of adiabatic polarization. This features were observed by Sarkar and Ghosh [6] who included the adiabatic and non-adiabatic polarization potential in the framework of close coupling approximation. These facts collectively establish the validity of our present approach in analysis of positron-lithium atom scattering in medium and high energy ranges.

In present method, continuum distorted wave functions have been used in the state wave function. In other words, it takes into account the effect of continuum on elastic channel. Moreover, in this method, perturbing potential is weaker than that of Born-approximation. Therefore, it is expected that results obtained by employing this method contain higher order terms. In this method, effective Z (atomic number) is calculated to suit the physical situations. The theoretical soundness of the present theory is well conceived. Since in the case of scattering of positrons by alkali atom, scattering parameters are sensitive to the polarization potential, so in the present investigation, polarization potential has been included. The polarization potential is the most effective near forward direction of differential cross sections. As a great deal of cancellation between polarization which is attractive and the static potential which is repulsive in nature , DCSPP near the forward direction are found to be less than DCSWP. The cancellation gives rise to minimum in curve. With the increase of energy, present results without polarization potential approach the first-Born results. This is expected due to the fact the effect of continuum is not appreciable with the enhancement of energy. The present result is consistent in this respect.

The suitability of this approach is being judged by employing it in case of other scattering problems. The work is in progress.

Acknowledgments

The authors are thankful to Professor A S Ghosh, IACS, Jadavpur, Calcutta-700 032 for valuable suggestions and discussion and also to Mr. P K Biswas, IACS for help in computational work.

References

[1] M S T Watts and J W Humberston *J. Phys.* **B.25** L 491 (1992)

[2] B R Junker *Phys. Rev.* **A2** 1552 (1975)

[3] A Nordsieck *Phys. Rev.* **A93** 785 (1954)

[4] S P Khare and Vijayshri *Indian J. Phys.* **62B** 483 (1988)

[5] S S Tayal, A N Tripathi and M K Shrivastava *Phys. Rev.* **A24** 1817 (1981)

[6] K P Sarkar and A S Ghosh *J. Phys.* **B22** 105 (1989)

[7] K C Mathur and R S Pundir *Internal Report IC/83/85/58* ICTP, Trieste, Italy (1983)

[8] S J Ward, M Horbatsch, R P Mc Eacharan and A D Stauffer *J. Phy* **B22** 1845 (1989)